LABORATORY MEASUREMENTS OF THE HYPERFINE STRUCTURE OF $H^{14}N^{12}C$ AND $D^{14}N^{12}C$

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ABSTRACT

The nuclear quadrupole hyperfine structure of $H^{14}N^{12}C$ and $D^{14}N^{12}C$ has been resolved in the laboratory for the first time using millimeter-wave absorption spectroscopy. The transient species were produced in a pulsed DC discharge nozzle, and Doppler broadening effects were minimized by propagating the millimeter waves coaxially with the supersonic molecular beam. New rest frequencies for the $J = 1$–0, $J = 2$–1, and $J = 3$–2 rotational transitions of the ground vibrational state were determined. The nuclear quadrupole coupling constants derived from the spectra are $(eQq)_N = 264.5 \pm 4.6$ kHz for $H^{14}N^{12}C$ and $(eQq)_N = 294.7 \pm 13.1$ kHz and $(eQq)_D = 261.9 \pm 14.5$ kHz for $D^{14}N^{12}C$.

Subject headings: astrochemistry — ISM: molecules — methods: laboratory — molecular data — radio lines: ISM

1. INTRODUCTION

The 1971 discovery (Snyder & Buhl 1971, 1972) of the U90.7 interstellar millimeter-wave emission line, which was later assigned to the $J = 1$–0 rotational transition of $H^{14}N^{12}C$ (Blackman et al. 1976; Creswell et al. 1976; Saykally et al. 1976), stimulated considerable interest in the astronomical community. Subsequent measurements of [HNC]/[HCN] and [DNC]/[HNC] abundance ratios have provided insights into the astrochemistry of dark clouds. In particular, measurements of the [HNC]/[HCN] abundance ratio imply that the abundance of HNC in some regions is comparable to that of HCN (Goldsmith et al. 1986; Harju 1989; Hirota et al. 1998; Irvine & Schloerb 1984; Schilke et al. 1992; Turner et al. 1997; Wootten et al. 1978), which is unexpected based on thermodynamics alone (HNC is 0.62 eV less stable than HCN). Those measurements suggest that the $HCNH^+ + e^-$ dissociative recombination reaction is a major source of HNC, although a decisive explanation for the relative overabundance of HNC remains to be established. The [DNC]/[HNC] abundance ratio is also significant: in dark cloud cores, [DNC]/[HNC] abundance ratios range from 0.008 to 0.122 (Hirota et al. 2001, 2003; Snell & Wootten 1979; Turner 2001), which is considerably higher than the cosmic [D]/[H] abundance ratio of about 10^{-5} (Wilson & Rood 1994). Deuterium fractionation into various molecules has been shown to be sensitive to a variety of physical conditions, including temperature and the degree of ionization.

Accurate measurements of abundance ratios require precise rest frequencies for observed transitions. Indeed, Turner (2001) has shown that neglect of hyperfine structure can lead to significant errors in astronomical observations of abundance ratios. Although precise rest frequencies are typically obtained in the laboratory, laboratory measurements on the chemically unstable HNC molecule are challenging. In 1963, Milligan & Jacox (1963) observed HNC in an argon matrix, but it was not until 1975 that Arrington & Ogryzlo (1975) observed a laboratory gas-phase spectrum. Since then, numerous groups have recorded microwave (Amano & Zelinger 2002; Blackman et al. 1976; Creswell et al. 1976; Okabayashi & Tanimoto 1993; Pearson et al. 1976; Saykally et al. 1976; Thorwirth et al. 2000) and infrared (Burkholder et al. 1987; Maki & Mellau 2001; Maki & Sams 1981; Nezu et al. 1998; Northrup et al. 1997; Winter & Jones 1982) spectra of HNC. The laboratory measurements, however, are not nearly as comprehensive as those

for the more stable HCN isomer, and in none of them is the HNC hyperfine structure resolved.

Here we present the first laboratory measurements of the resolved hyperfine structure of $H^{14}N^{12}C$ and $D^{14}N^{12}C$ in the ground vibrational state.

2. EXPERIMENTAL

These measurements are performed in a coaxial millimeter-wave pulsed discharge jet spectrometer, which provides better resolution than the conventional orthogonal geometry by minimizing Doppler and transit time broadening. The design of the spectrometer is similar to that of Walker & McKellar (2001) and McElmurry et al. (2003) with the addition of a pulsed discharge nozzle (Steeves et al. 2005), which extends the capabilities of the coaxial millimeter-wave jet spectrometer to rotationally cold transient species. Here HNC (DNC) is generated with a mixture of 2% CH_3CN (CD_3CN) in Ne. The pulsed valve operates at 10 Hz with a backing pressure of 3 atm, a pulse duration of approximately 300 μs, a negative discharge voltage of 1.5 kV, and a discharge pulse length of 200 μs centered on the gas pulse. The discharge nozzle is mounted at the rear of an aluminum rooftop reflector that has a small hole (∼1 cm diameter) at the center for the molecular beam.

The millimeter-wave radiation is produced by a W-band (72–106 GHz) Gunn oscillator (J. E. Carlstrom Co.) that is phase-locked (XL Microwave 800A) to the 10th harmonic of a microwave synthesizer (HP 8673E) and coupled through waveguide components to a calibrated attenuator (Hitachi W9513). Higher frequencies are generated by doubling (144–212 GHz) and tripling (216–318 GHz) the output of the Gunn oscillator in Schottky diode multipliers (Virginia Diodes). The radiation is emitted into free space through a standard gain pyramidal horn and passed through a wire-grid polarizer oriented to pass the linearly polarized millimeter-wave radiation. A polytetrafluoroethylene lens ($f = 30$ cm) is used to roughly collimate the millimeter-wave radiation, which is counterpropagated with the molecular beam and directed onto the rooftop reflector oriented at 45° with respect to the polarization of the millimeter waves. The rooftop reflector rotates the millimeter-wave polarization by 90° and reflects the millimeter-wave radiation back onto itself, making a second pass of the vacuum chamber. The millimeter-wave radiation is focused by the PTFE lens and finally reflected by the polarizer onto a liquid helium-cooled InSb hot electron bo-

TABLE 1
TRANSITION FREQUENCIES OF H^{14}N^{12}C

J'–J''	F'–F''	Observed (MHz)	Observed−Calculated (MHz)
1–0	0–1	90663.417	0.000
	2–1	90663.556	−0.002
	1–1	90663.622	−0.001
2–1	1–1	181324.585	−0.001
	2–1	181324.729[a]	−0.005
	3–2	181324.729[a]	−0.005
	1–0	181324.792[a]	−0.002
	2–2	181324.792[a]	−0.002
3–2	3–2	271981.111[a]	−0.003
	4–3	271981.111[a]	−0.003
	2–1	271981.111[a]	−0.003

[a] Unresolved feature.

lometer (Cochise Instruments). The bolometer output is digitized with a 500 MHz oscilloscope (Lecroy LC334A) and transferred to a computer for storage.

To record an absorption spectrum, the phase-lock loop reference (HP 3336B) is scanned in 2 kHz steps around a center frequency of 35 MHz. The coaxial geometry of the millimeter-wave radiation and the molecular beam results in two Doppler-split peaks, the frequencies of which are averaged to determine the rest frequency. The separation of the peaks indicates that the molecular beam speed is about 890 m s^{-1}. The spectrometer was calibrated by measuring several rotational transitions of OCS and HCN (Müller et al. 2005). The uncertainty in the absolute frequencies for the measured transitions is ± 5 kHz for the $J = 1$–0 transitions and ± 10 kHz for the $J = 2$–1 and $J = 3$–2 transitions, whereas the uncertainty of the hyperfine splitting in a single rotational transition is ± 2 kHz.

3. RESULTS AND ANALYSIS

The hyperfine structure in H^{14}N^{12}C is dominated by the interaction of the valence shell electrons with the electric quadrupole moment of the ^{14}N ($I_N = 1$) nucleus. Although generally much smaller, the nuclear spin-rotation interaction, which is caused by the interaction of rotating charged particles (electrons and nuclei) with the magnetic moment of the ^{14}N atom, also contributes to the hyperfine structure. These interactions cause the lowest rotational transition $J = 1$–0 of H^{14}N^{12}C to be split into three components and the higher rotational transitions to be split into six components.

The hyperfine structure of D^{14}N^{12}C, on the other hand, is substantially more complicated because of the additional coupling of the D ($I_D = 1$) nucleus. This coupling gives rise to a septet in the $J = 1$–0 transition and over 40 incompletely resolved lines in the higher J rotational transitions. The Hamiltonian for the hyperfine structure of D^{14}N^{12}C is

$$H_{hfs} = \frac{(eQq)_N}{2I_N(2I_N-1)(2J-1)(2J+3)}$$

$$\times [3(\mathbf{I}_N\cdot\mathbf{J})^2 + (3/2)(\mathbf{I}_N\cdot\mathbf{J}) - I_N^2 J^2] + C_N(\mathbf{I}_N\cdot\mathbf{J})$$

$$+ \frac{(eQq)_D}{2I_D(2I_D-1)(2J-1)(2J+3)}$$

$$\times [3(\mathbf{I}_D\cdot\mathbf{J})^2 + (3/2)(\mathbf{I}_D\cdot\mathbf{J}) - I_D^2 J^2] + C_D(\mathbf{I}_D\cdot\mathbf{J}),$$

where $(eQq)_N$ and $(eQq)_D$ are the nuclear quadrupole coupling constants and C_N and C_D are the spin-rotation constants of nitrogen and deuterium, respectively. Although analytical expres-

TABLE 2
TRANSITION FREQUENCIES OF D^{14}N^{12}C

J'–J''	F'_N–F''_N	F'–F''	Observed (MHz)	Observed−Calculated (MHz)
1–0	0–1	1–0, 1, 2	76305.511	0.000
	2–1	1–0, 1, 2	76305.630	0.000
	2–1	3–2	76305.678	0.001
	2–1	2–1, 2	76305.717	0.000
	1–1	1–0, 1, 2	76305.790[a]	−0.002
	1–1	2–1, 2	76305.790[a]	−0.002
	1–1	0–1	76305.836	0.002
2–1	1–1	2–2	152609.569[a]	0.005
	1–1	2–1	152609.569[a]	0.005
	1–1	1–2	152609.569[a]	0.005
	1–1	1–1	152609.569[a]	0.005
	2–1	3–2	152609.746[a]	−0.002
	3–2	4–3	152609.746[a]	−0.002
	3–2	2–1	152609.746[a]	−0.002
	3–2	3–2	152609.746[a]	−0.002
	2–1	2–2	152609.746[a]	−0.002
	2–1	2–1	152609.746[a]	−0.002
	1–0	2–1	152609.845[a]	−0.003
	2–2	3–3	152609.845[a]	−0.003
	1–0	1–1	152609.845[a]	−0.003
	2–2	1–1	152609.845[a]	−0.003
3–2	3–2	2–1	228910.481[a]	0.001
	3–2	4–3	228910.481[a]	0.001
	4–3	5–4	228910.481[a]	0.001
	4–3	3–2	228910.481[a]	0.001
	4–3	4–3	228910.481[a]	0.001
	3–2	3–2	228910.481[a]	0.001
	2–1	3–2	228910.481[a]	0.001

[a] Unresolved feature.

sions for hyperfine energy levels are well known for molecules containing a single-coupling ($I > \frac{1}{2}$) nucleus (Gordy & Cook 1984), such as H^{14}N^{12}C, the full secular determinant must be solved for molecules containing multiple-coupling nuclei, particularly when the values of the quadrupole coupling constants are comparable in magnitude, as in D^{14}N^{12}C (Bardeen & Townes 1948; Thaddeus et al. 1964). Here we have used the SPFIT program (Pickett 1991) to perform a global fit of the rotational transitions of H^{14}N^{12}C and D^{14}N^{12}C. In this global fit, we used the data obtained from the present work, which includes resolved and partially resolved hyperfine lines up to 275 GHz. For the H^{14}N^{12}C rotational transitions above 275 GHz, we used the hyperfine free data of Okabayashi & Tanimoto (1993) for the $J = 4$–3 transition, the data of Amano & Zelinger (2002) for the $J = 7$–6 transition, and the data of Thorwirth et al. (2000) for the $J = 5$–4, $J = 6$–5, $J = 8$–7, $J = 9$–8, $J = 10$–9, and $J = 22$–21 transitions. For the D^{14}N^{12}C transitions above 275 GHz, we used the data of Brünken et al. (2006). The experimental transition frequencies from the present work are shown in Tables 1 and 2, and the derived spectroscopic constants are shown in Table 3 along with previously published values. In analogy to the hyperfine assignments of D^{12}C^{14}N (DeLucia & Gordy 1969), we have used the sequential spin-coupling scheme to label the D^{14}N^{12}C transitions:

$$\mathbf{J} + \mathbf{I}_N = \mathbf{F}_N,$$

$$\mathbf{F}_N + \mathbf{I}_D = \mathbf{F}.$$

The experimental data were not sufficient to accurately determine C_D. Previous measurements of C_D in D^{12}C^{14}N (DeLucia & Gordy 1969) have shown that it is small (-0.6 ± 0.3 kHz), and we do not expect it to change significantly in D^{14}N^{12}C. As

Parameter	$H^{14}N^{12}C$ (Present Work)	$H^{14}N^{12}C$ Hyperfine Free[a]	$H^{14}N^{13}C$ (Turner 2001)	$D^{14}N^{12}C$ (Present Work)	$D^{14}N^{12}C$ (Brünken et al. 2006)	$D^{14}N^{12}C$ (Turner 2001)
B (MHz)	45331.98160(52)	45331.98415(79)	...[b]	38152.98807(36)	38152.98692(156)	...[b]
D (kHz)	99.8097(45)	99.8286(63)	...[b]	68.97119(281)	0.0689649(87)	...[b]
H (Hz)	0.1458(57)	0.1682(78)	...[b]	0.1984(37)	0.1925(82)	...[b]
$(eQq)_N$ (kHz)	264.5(46)	...[b]	276(21)	294.7(131)	...[b]	378.7(260)
C_N (kHz)	7.15(109)	...[b]	10.5(43)	5.01(99)	...[b]	...[b]
$(eQq)_D$ (kHz)	...	...	...	261.9(145)	...[b]	111(154)

NOTES.—Values in parentheses represent one standard deviation (1 σ) in the units of the last digit. The errors produced in the SPFIT program (Pickett 1991) were converted to standard errors using the PFORM program from http://info.ifpan.edu.pl/~kisiel/prospe.htm.
[a] Data in fit: $J = 1–0$ (Saykally et al. 1976); $J = 2–1$ (Creswell et al. 1976); $J = 3–2$, $J = 4–3$ (Okabayashi & Tanimoto 1993); $J = 5–4$, $J = 6–5$, $J = 8–7$, $J = 9–8$, $J = 10–9$, $J = 22–21$ (Thorwirth et al. 2000); $J = 7–6$ (Amano & Zelinger 2002).
[b] Not determined in fit.

a consequence, we have omitted it from the fit. The omission of C_D did not affect the quality of the fit.

Figure 1a shows the experimental millimeter-wave spectrum of $H^{14}N^{12}C$ ($J = 1–0$) and a simulation based on molecular constants determined from the fit. Positive and negative Doppler shifts, corresponding to a molecular beam speed of 890 m s^{-1}, are added to the calculated line positions, and the doubled lines are convoluted with a Lorentzian line shape of 50 kHz width. The experimental resolution is sufficient to resolve all three hy-

FIG. 1.—(a) $H^{14}N^{12}C$ ($J = 1–0$) and (b) $D^{14}N^{12}C$ ($J = 1–0$) experimental spectra (circles). The coaxial geometry results in two Doppler-split peaks, the frequencies of which are averaged to determine the rest frequency. The stick spectrum and simulation (solid line) are based on the molecular constants determined from the fit, assuming Lorentzian line shapes of 50 kHz and a molecular beam speed of 890 m s^{-1}.

perfine components in the $H^{14}N^{12}C$ ($J = 1–0$) rotational transition. The hyperfine transitions of the $J = 2–1$ and $J = 3–2$ rotational transitions, however, are not fully resolved. This failure to resolve fully all of the hyperfine components is due in part to the decreased separation between hyperfine lines in higher rotational transitions and the presence of six lines rather than three. The primary reason, however, is the degradation of experimental resolution caused by the linear frequency dependence of the Doppler line width. Thus, at 90 GHz, the experimental line shapes are nearly Lorentzian with line widths of about 50 kHz, whereas at 180 GHz and 270 GHz, the line shapes are predominantly Gaussian with line widths of about 100 kHz and 180 kHz, respectively.

The experimental millimeter-wave spectrum of $D^{14}N^{12}C$ ($J = 1–0$) and the corresponding simulation is shown in Figure 1b. As noted above, the nuclear spin of deuterium causes additional splitting, resulting in seven lines instead of three for the $J = 1–0$ rotational transition. Although the experimental resolution is not sufficient to fully resolve all members of the $F_N = 1–1$ triplet, the remaining lines can be distinguished. For the $J = 2–1$ and $J = 3–2$ transitions, the increased Doppler broadening at higher frequencies conceals all deuterium splitting effects and the profiles of the higher rotational transitions are similar to those of $H^{14}N^{12}C$.

4. DISCUSSION

The nuclear quadrupole constant of $H^{14}N^{12}C$, as measured in this work, is $(eQq)_N = 264.5 \pm 4.6$ kHz. It has the opposite sign and is considerably smaller than the nuclear quadrupole constant of the more stable $H^{12}C^{14}N$ isomer, $(eQq)_N = -4709.03 \pm 1.62$ kHz (Ahrens et al. 2002). The small value of $(eQq)_N$ for $H^{14}N^{12}C$ arises from the decreased electric field gradient at the central ^{14}N nucleus and is typical of other isonitriles, such as CH_3NC and $HCCNC$, which have nuclear quadrupole constants of 489.4 ± 0.4 kHz (Kukolich 1972) and 946.4 ± 1.9 kHz (Krüger et al. 1991), respectively. The most recent ab initio calculations (Pd & Chandra 2001) on $H^{14}N^{12}C$ also predict a small nuclear quadrupole coupling constant, -313 kHz $\geq (eQq)_N \geq -288$ kHz, but of the wrong sign.

Although the hyperfine structure of $H^{14}N^{12}C$ has not hitherto been resolved in the laboratory, partially resolved hyperfine structure has been observed in millimeter emission measurements of $H^{14}N^{12}C$ in interstellar dark clouds. Snyder et al. (1977) first estimated the quadrupole coupling constant of $H^{14}N^{12}C$ from those observations, but self-absorption (Watson et al. 1978) of the strongest component, $F = 2–1$, led to incorrect assignments of the hyperfine structure and a quadrupole coupling constant with the wrong sign. Later, Frerking et al.
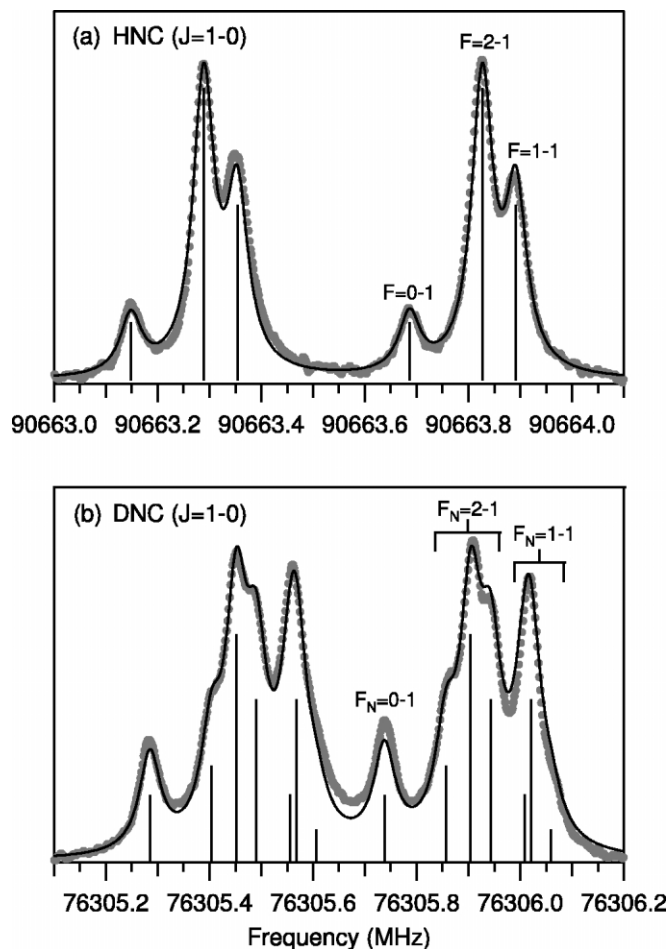
(1979) gave improved estimates of the hyperfine transition frequencies and the nuclear quadrupole constant of $H^{14}N^{12}C$ and $H^{14}N^{13}C$. Those estimates are updated by the more recent measurements of Turner (2001), which are shown in Table 3. Although the $H^{14}N^{13}C$ astronomical value for $(eQq)_N$ is in good agreement with our laboratory measurements, the $D^{14}N^{12}C$ astronomical values for both $(eQq)_N$ and $(eQq)_D$ are not. The discrepancy is most likely a consequence of the insufficient resolution in the astronomical spectra, which prevents an accurate determination of the nuclear quadrupole constants.

Also shown in Table 3 are the $H^{14}N^{12}C$ and $D^{14}N^{12}C$ molecular constants determined from the most precise hyperfine free data in the literature. A comparison of the B, D, and H rotational constants indicate that the $D^{14}N^{12}C$ constants from the present work agree within 1 σ with the values obtained by Brünken et al. (2006). The rotational constants of $H^{14}N^{12}C$, however, lie just outside of the 1 σ ranges of the fit to the hyperfine free data set. The discrepancy arises primarily from the difference in our value of the $J = 3$–2 rotational transition and that of Okabayashi & Tanimoto (1993) as well as the

increased weighting of the lower rotational transitions in the fit from the reduced uncertainty in our measurements.

The improved resolution of the coaxial millimeter-wave discharge jet spectrometer has permitted the hyperfine structure of $H^{14}N^{12}C$ and $D^{14}N^{12}C$ to be resolved for the first time in the laboratory. The updated rest frequencies should aid astronomical measurements of [HCN]/[HNC] and [DNC]/[HNC] abundance ratios, particularly when the hyperfine structure is incompletely resolved or suffers from self-absorption.

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